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Kinetics of crystalline nuclei growth in glassy systems

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Abstract

© 2017 the Owner Societies. In this work, we study crystalline nuclei growth in glassy systems, focusing primarily on the early stages of the process, during which the size of a growing nucleus is still comparable with the critical size. On the basis of molecular dynamics simulation results obtained for two crystallizing glassy systems, we evaluate the growth laws of the crystalline nuclei and the parameters of the growth kinetics at temperatures corresponding to deep supercooling; herein, a statistical treatment of the simulation results is carried out using the mean-first-passage-time method. It is found that for the considered systems at different temperatures, the crystal growth laws that were rescaled onto the waiting times of the critically-sized nuclei follow a unified dependence, and can significantly simplify the theoretical description of the post-nucleation growth of crystalline nuclei. The evaluated size-dependent growth rates are characterized by a transition to the steady-state growth regime, which depends on the temperature and occurs in the glassy systems when the size of a growing nucleus becomes two-three times larger than the critical size. It is suggested that the temperature dependencies of the crystal growth rate characteristics should be considered by using the reduced temperature scale T. Thus, it is revealed that the scaled values of the crystal growth rate characteristics (namely, the steady-state growth rate and the attachment rate for the critically-sized nucleus) as functions of the reduced temperature T for glassy systems follow unified power-law dependencies. This finding is supported by the available simulation results; the correspondence with the experimental data for the crystal growth rates in glassy systems at temperatures near the glass transition is also discussed.

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